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PTO-1590 (9-90)

July 17, 2002

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REP G1=(1-2) C VAR G2=12/13 NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
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DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E2 N AT 12
ECOUNT IS E5 C E4 N AT 13

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L6 2222803 SEA FILE=REGISTRY ABB=ON PLU=ON NC4/ES OR NC5/ES OR NC6/ES L7 56091 SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND (NCNC3/ES OR NCNC2-NCN

C3/ES)

L9 55 SEA FILE=REGISTRY SUB=L7 SSS FUL L5
L10 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L9

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L10 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 2001:710917 HCAPLUS

DOCUMENT NUMBER: 136:216993

TITLE: Synthesis and binding affinity of a chiral PNA

analogue

AUTHOR(S): Li, Ying; Jin, Tao; Liu, Keliang

CORPORATE SOURCE: Beijing Institute of Pharmacology and Toxicology,

Beijing, 100850, Peop. Rep. China

SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2001),

20(9), 1705-1721

CODEN: NNNAFY; ISSN: 1525-7770

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

AB The synthesis of a chiral peptide nucleic acid (PNA), which is composed of N-aminoethyl-cis-4-nucleobase-L-proline units, was described. The chiral PNA monomers contg. all four nucleobases (A, T, C and G) were stereoselectively prepd. using key intermediate (I), prepd. in two steps from (CH3)3COC(0)NH(CH2)2Br and trans-L-hydroxyproline Et ester hydrochloride. The x-ray diffraction data from a single crystal confirmed the configuration of a key intermediate. Binding activity of the oligomers with their complementary DNA targets was also investigated.

IT 386212-22-2P 386212-24-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. of cis-L-proline-based PNA oligomers and their hybridization characteristics with DNA)

RN 386212-22-2 HCAPLUS

Adenosine, 2'-deoxyadenylyl-(3'.fwdarw.5')-thymidylyl-2'-deoxyadenylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-2'-deoxy-, complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl)-Lys-NH2 (1:1) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 386212-21-1 CMF C80 H101 N28 O46 P7

PAGE 1-A

PAGE 1-B

PAGE 3-A

CM 2

CRN 386212-19-7

CMF C102 H139 N47 O17

PAGE 1-A

PAGE 1-B

PAGE 3-A

RN 386212-24-4 HCAPLUS
CN Adenosine, 2'-deoxyadenylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-

2'-deoxy-, complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl)-L-prolyl-L-prolyl-L-prolyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl)-L-prolyl)-Lys-NH2 (1:1) (9CI) (CA INDEX NAME)

CM 1

NH2

CRN 386212-23-3

CMF C80 H101 N28 O46 P7

PAGE 1-B

PAGE 2-A

PAGE 2-B

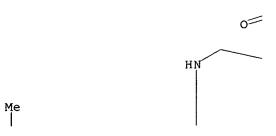
CM 2

CRN 386212-19-7

CMF C102 H139 N47 O17

 ${\tt Absolute \ stereochemistry.}$

PAGE 1-A



PAGE 1-A

PAGE 1-B

PAGE 2-B

H₂N

PAGE 3-A

IT 253307-71-0P 340961-43-5P 340961-45-7P 371970-41-1P 386212-13-1P 386212-14-2P 386212-15-3P 386212-16-4P 386212-17-5P 386212-18-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cis-L-proline-based PNA oligomers and their hybridization characteristics with DNA)

RN 253307-71-0 HCAPLUS

CN L-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 340961-43-5 HCAPLUS

CN L-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 340961-45-7 HCAPLUS

CN L-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, (4S)- (9CI) (CA INDEX NAME)

RN 371970-41-1 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 386212-13-1 HCAPLUS

CN L-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 386212-14-2 HCAPLUS

CN L-Proline, 4-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 386212-15-3 HCAPLUS

CN L-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, ethyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 386212-16-4 HCAPLUS

CN L-Proline, 4-(6-amino-9H-purin-9-yl)-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 386212-17-5 HCAPLUS

CN L-Proline, 4-[6-(dibenzoylamino)-9H-purin-9-yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 386212-18-6 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 386212-19-7P 386212-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of cis-L-proline-based PNA oligomers and their hybridization characteristics with DNA)

RN 386212-19-7 HCAPLUS

CN Peptide nucleic acid, (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl)-L-prolyl)-L-prolyl)-Lys-NH2 (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

H₂N

RN 386212-20-0 HCAPLUS
CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-7H-purin-7yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester, (4S)(9CI) (CA INDEX NAME)

PAGE 3-A

Absolute stereochemistry.

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS 20 REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

2001:675176 HCAPLUS

DOCUMENT NUMBER:

135:354283

TITLE:

Engineering preferences of hairpin PNA binding to

complementary DNA: effect of N7G in aeg/aep PNA

backbone

AUTHOR(S):

Kumar, V. A.; D'Costa, M.; Ganesh, K. N.

CORPORATE SOURCE:

Division of Organic Chemistry (Synthesis), National

Chemical Laboratory, Pune, India

SOURCE:

Nucleosides, Nucleotides & Nucleic Acids (2001),

20(4-7), 1187-1191

CODEN: NNNAFY; ISSN: 1525-7770

PUBLISHER:

Marcel Dekker, Inc.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Aminoethylgylcyl peptide nucleic acid (aegPNA) and aminoethylpropyl peptide nucleic acid (aepPNA) monomeric units bearing the N7-guanine nucleobase as a substitute for protonated cytosine (C+) have been shown to bind to a GC base-pair of a duplex in a pH-independent manner when placed in the third strand. The aepPNA backbone exerts a preference for binding in the antiparallel Hoogsteen mode over the parallel Hoogsteen mode.

340961-45-7P 371970-41-1P ΙT

RL: PNU (Preparation, unclassified); PREP (Preparation) (recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

340961-45-7 HCAPLUS RN

L-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-CN [[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, (4S)- (9CI) (CA INDEX NAME)

RN 371970-41-1 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 340961-34-4P 371970-40-0P

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

RN 340961-34-4 HCAPLUS

CN L-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 371970-40-0 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2002 ACS 2001:238460 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 135:107554

TITLE: Aminoethylprolyl (aep) PNA: Mixed Purine/Pyrimidine

Oligomers and Binding Orientation Preferences for

PNA: DNA Duplex Formation

D'Costa, Moneesha; Kumar, Vaijayanti; Ganesh, Krishna AUTHOR(S):

Division of Organic Chemistry (Synthesis), National CORPORATE SOURCE:

Chemical Laboratory, Pune, 411008, India SOURCE:

Organic Letters (2001), 3(9), 1281-1284

CODEN: ORLEF7; ISSN: 1523-7060 PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal English LANGUAGE:

GI

AB The synthesis of (2S,4S) - and (2R,4S) -aepPNA monomers (I; Base = adenine, quanine, and cytosine) and their incorporation at appropriate positions into aegPNA sequence leads to mixed aeg-aep backbone/mixed nucleobase PNAs. Beginning with (2S,4R)-4-hydroxyl-N-(N-Boc-aminoethyl)-L-proline Me ester (Boc = (CH3)3COC(O)-) or its 2R,4R isomer, the hydroxy group was mesylated, and the product reacted with protected Base to give Boc-protected Me esters of I, which, with the similar thymidyl deriv., were used to synthesize four PNAs of the sequence H-GTagAtcACT-NH(CH2)2CO2H, where lower case letters indicate position of a single

substitution. The thermal stabilities of the derived duplexes with DNA are found to be dependent on nucleobase and backbone stereochem.

IT 253307-71-0 253307-76-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. and hybridization studies of mixed base PNAs contg.

aminoethylprolyl backbone monomers)

RN 253307-71-0 HCAPLUS

CN L-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 253307-76-5 HCAPLUS

CN D-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 340961-33-3P 340961-34-4P 340961-36-6P

340961-40-2P 340961-41-3P 340961-42-4P

340961-43-5P 340961-44-6P 340961-45-7P

340961-46-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and hybridization studies of mixed base PNAs contg.

aminoethylprolyl backbone monomers)

RN 340961-33-3 HCAPLUS

CN L-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CFINDEX NAME)

RN 340961-34-4 HCAPLUS

CN L-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 340961-36-6 HCAPLUS

CN L-Proline, 4-(2-amino-6-chloro-9H-purin-9-yl)-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

340961-40-2 HCAPLUS RN

D-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[(1,1-CN dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

340961-41-3 HCAPLUS RN

D-Proline, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-1-[2-[[(1,1-CN dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

340961-42-4 HCAPLUS RN

D-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-CN [[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, (4S)- (9CI) (CA INDEX NAME)

340961-43-5 HCAPLUS RN

L-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[(1,1-CN dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

340961-44-6 HCAPLUS RN

L-Proline, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-1-[2-[[(1,1-CN dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

340961-45-7 HCAPLUS RN

L-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-dimethylethoxy][[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, (4S)- (9CI) (CA INDEX NAME)

09/666,144

340961-46-8 HCAPLUS RN

L-Proline, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-1-[2-[[(1,1dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CA CN INDEX NAME)

Absolute stereochemistry.

340961-35-5P 340961-37-7P 340961-38-8P ΙT 340961-39-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and hybridization studies of mixed base PNAs contg. aminoethylprolyl backbone monomers)

340961-35-5 HCAPLUS

L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-7H-purin-7-RNyl]-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-CN (9CI) (CA INDEX NAME)

Absolute stereochemistry.

340961-37-7 HCAPLUS RN

D-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[(1,1dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CA CN INDEX NAME)

RN 340961-38-8 HCAPLUS

CN D-Proline, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 340961-39-9 HCAPLUS

CN D-Proline, 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 2000:844932 HCAPLUS

DOCUMENT NUMBER: 134:147837

TITLE: Synthesis and properties of chiral peptide nucleic

acids with a N-aminoethyl-D-proline backbone

AUTHOR(S): Vilaivan, Tirayut; Khongdeesameor, Chanchai;

Harnyuttanakorn, Pongchai; Westwell, Martin S.; Lowe,

Gordon

CORPORATE SOURCE: Organic Synthesis Research Unit, Department of

Chemistry, Faculty of Science, Chulalongkorn

University, Bangkok, 10330, Thailand

SOURCE: Bioorganic & Medicinal Chemistry Letters (2000),

10(22), 2541-2545

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:147837

AB A synthon of D-proline substituted at the 4-position by thymine and at N by a flexible aminoethyl linker, has been used to prep. a novel chiral peptide nucleic acid (cPNA) with (2R,4R) stereochem. using solid phase methodol. The homothymine decamer cPNA binds to complementary polyadenylic acid to form 2:1 hybrid with high affinity and specificity according to UV and CD studies, whereas no binding to the corresponding polydeoxyadenylic acid was obsd.

IT 318515-52-5P 318515-53-6P 318515-54-7P 318515-55-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(solid phase synthesis and properties of chiral peptide nucleic acids with a aminoethylproline backbone)

RN 318515-52-5 HCAPLUS

CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)1-[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]ethyl]-, diphenylmethyl
ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 318515-53-6 HCAPLUS

CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)1-[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]ethyl]-, monohydrochloride,
(4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

HCl

RN 318515-54-7 HCAPLUS

CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)1-[2-[[(4-nitrophenyl)sulfonyl]amino]ethyl]-, diphenylmethyl ester, (4R)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 318515-55-8 HCAPLUS

CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)1-[2-[((1,1-dimethylethoxy)carbonyl]amino]ethyl]-, diphenylmethyl ester,
(4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 318515-56-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid phase synthesis and properties of chiral peptide nucleic acids with a aminoethylproline backbone)

RN 318515-56-9 HCAPLUS

CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1999:663052 HCAPLUS

DOCUMENT NUMBER:

132:251401

TITLE:

Aminoethylprolyl Peptide Nucleic Acids (aepPNA):

Chiral PNA Analogues That Form Highly Stable

DNA:aepPNA2 Triplexes

AUTHOR(S):

D'Costa, Moneesha; Kumar, Vaijayanti A.; Ganesh,

Krishna N.

CORPORATE SOURCE:

Division of Organic Chemistry (Synthesis), National

Chemical Laboratory, Pune, 411008, India

Organic Letters (1999), 1(10), 1513-1516 SOURCE:

CODEN: ORLEF7; ISSN: 1523-7060

American Chemical Society PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

The replacement of the glycyl component in the peptide nucleic acid (PNA) AΒ backbone by a prolyl unit bearing a nucleobase leads to the aminoethylprolyl (aep) PNAs, which are chiral and cationic. The homo-oligomeric aepPNA binds to complementary DNA sequences with high affinity and sequence specificity, forming highly stable triplexes.

253307-69-6P 253307-71-0P 253307-74-3P IT

253307-76-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of in the synthesis of aminoethylprolyl peptide nucleic acids)

253307-69-6 HCAPLUS RN

L-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-CN 1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

253307-71-0 HCAPLUS RN

L-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrimidinyl)-1-[2-methyl-2,4-dioxo-1(H)-pyrCN [[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

253307-74-3 HCAPLUS RN

D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-CN

1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 253307-76-5 HCAPLUS

CN D-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

262614-79-9P 262614-81-3P 262615-03-2P IT 262615-29-2P 262615-33-8P 262615-36-1P 262615-38-3P 262615-58-7P 262615-78-1P 262615-79-2P 262615-84-9P 262615-88-3P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and triplex stability of) 262614-79-9 HCAPLUS RN DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid CN (H-T-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1)1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME) CM 1 262408-13-9 CRN Unspecified CMF CCI MAN CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253307-78-7

CMF C92 H121 N33 O33

PAGE 1-C

RN 262614-81-3 HCAPLUS

CN DNA, d(G-C-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid (H-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9 CMF Unspecified CCI MAN

CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253307-80-1 CMF C92 H121 N33 O33

PAGE 1-C

RN 262615-03-2 HCAPLUS

CN DNA, d(G-C-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9 CMF Unspecified CCI MAN CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253307-82-3 CMF C93 H123 N33 O32

PAGE 1-C

PAGE 2-A

PAGE 2-B

262615-29-2 HCAPLUS RN

DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-1)CN pyrimidinyl)-Pro-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-

July 17, 2002

09/666,144

dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253307-84-5

CMF C93 H123 N33 O32

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

PAGE 2-A

PAGE 2-B

RN 262615-33-8 HCAPLUS

CN DNA, d(G-C-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9 CMF Unspecified CCI MAN CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-10-8 CMF C95 H127 N33 O30

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-B

- 262615-36-1 HCAPLUS RN
- DNA, d(G-C-A-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1) CN pyrimidinyl) -Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-

 $\label{eq:continuous} $1(2H) - \text{pyrimidinyl} - \text{Pro-T-}(4S) - 1 - (2-\text{aminoethyl}) - 4 - (3, 4-\text{dihydro-5-methyl-2}, 4-\text{dioxo-1}(2H) - \text{pyrimidinyl}) - \text{Pro-T-}(4S) - 1 - (2-\text{aminoethyl}) - 4 - (3, 4-\text{dihydro-5-methyl-2}, 4-\text{dioxo-1}(2H) - \text{pyrimidinyl}) - \text{Pro}) - \text{Bal-OH} (1:2) (9CI) (CA INDEX NAME)$

CM 1

CRN 262408-13-9 CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-11-9 CMF C95 H127 N33 O30

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

=0

PAGE 2-A

RN 262615-38-3 HCAPLUS

CN DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-12-0

CMF C99 H135 N33 O26

PAGE 1-A

PAGE 1-B

PAGE 3-A

RN 262615-58-7 HCAPLUS

CN DNA, d(G-C-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-

 $\label{eq:control_loss} 1 \ (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - Pro- (4S) - 1- (2-aminoethyl) - 4- (3, 4-dihydro-5-methyl-2, 4-dioxo-1 (2H) - pyrimidinyl) - 4- (3, 4-dihydr$

CM 1

CRN 262408-13-9 CMF Unspecified CCI MAN CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-13-1 CMF C99 H135 N33 O26

Absolute stereochemistry.

PAGE 1-A

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PAGE 2-B

PAGE 3-A

H₂N

RN 262615-78-1 HCAPLUS

CN DNA, d(G-C-A-A-A-T-A-A-A-C-G), complex with peptide nucleic acid (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-14-0 CMF Unspecified CCI MAN CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-10-8 CMF C95 H127 N33 O30

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

PAGE 1-C

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PAGE 2-B

RN 262615-79-2 HCAPLUS

CN DNA, d(G-C-A-A-A-T-A-A-A-C-G), complex with peptide nucleic acid (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-

CM 1

CRN 262408-14-0

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-11-9

CMF C95 H127 N33 O30

Absolute stereochemistry.

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

PAGE 1-C

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PAGE 2-A

RN 262615-84-9 HCAPLUS

CN DNA, d(G-C-A-A-A-T-A-A-A-C-G), complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-14-0

CMF Unspecified

CCI MAN

CDES NS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-12-0

CMF C99 H135 N33 O26

PAGE 1-A

PAGE 1-B

H₂N 0

262615-88-3 HCAPLUS

RN

N DNA, d(G-C-A-A-A-T-A-A-A-C-G), complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-

PAGE 3-A

 $\begin{array}{lll} 1 & (2H) - pyrimidinyl) - Pro-(4S) - 1 - (2-aminoethyl) - 4 - (3, 4-dihydro-5-methyl-2, 4-dioxo-1(2H) - pyrimidinyl) - Pro-(4S) - 1 - (2-aminoethyl) - 4 - (3, 4-dihydro-5-methyl-2, 4-dioxo-1(2H) - pyrimidinyl) - Pro-(4S) - 1 - (2-aminoethyl) - 4 - (3, 4-dihydro-5-methyl-2, 4-dioxo-1(2H) - pyrimidinyl) - Pro-(4S) - 1 - (2-aminoethyl) - 4 - (3, 4-dihydro-5-methyl-2, 4-dioxo-1(2H) - pyrimidinyl) - Pro-(4S) - 1 - (2-aminoethyl) - 4 - (3, 4-dihydro-5-methyl-2, 4-dioxo-1(2H) - pyrimidinyl) - Pro-(4S) - 1 - (2-aminoethyl) - 4 - (3, 4-dihydro-5-methyl-2, 4-dioxo-1(2H) - pyrimidinyl) - Pro) - Bal-OH (1:2) (9CI) (CA INDEX NAME) \\ \end{array}$

CM 1

CRN 262408-14-0 CMF Unspecified CCI MAN CDES NS

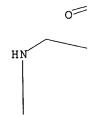
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-13-1 CMF C99 H135 N33 O26

Absolute stereochemistry.

PAGE 1-A



Мe

PAGE 2-B

PAGE 3-A

H₂N_

IT 253307-78-7P 253307-80-1P 253307-82-3P 253307-84-5P 253342-10-8P 253342-11-9P 253342-12-0P 253342-13-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and triplex-forming properties of as chiral PNA analogs) 253307-78-7 HCAPLUS

RN 253307-78-7 HCAPLUS

CN Peptide nucleic acid, (H-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (9CI) (CA INDEX NAME)

PAGE 1-C

253307-80-1 HCAPLUS RN

Peptide nucleic acid, (H-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-CNdihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (9CI) (CA INDEX NAME)

PAGE 1-C

253307-82-3 HCAPLUS RN

Peptide nucleic acid, (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (9CI) CN (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

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 R
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RN 253307-84-5 HCAPLUS

CN Peptide nucleic acid, (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (9CI) (CA INDEX NAME)

Searched by Paul Schulwitz (703)305-1954

PAGE 1-C

253342-10-8 HCAPLUS

RN

CN Peptide nucleic acid, (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-1-(2-aminoethyl)-4-(3,4-dioxo-1(2H)-pyrimidinyl)-1-(2-aminoethyl)-1-(2-aminoethyl)-1-(2-aminoethyl)-1-(2-aminoethyl)-1-(2-aminoethyl)-1-(2-aminoethyl)-1-(2-aminoethyl)-1-(3,4-dioxo-1(2H)-pyrimidinyl)-1-(3,4-dioxo-1(2H)-pyrimidinyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-aminoethyl)-1-(3-ami

PAGE 2-B

dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

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PAGE 1-C

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PAGE 2-A

PAGE 2-B

RN 253342-11-9 HCAPLUS

CN Peptide nucleic acid, (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (9CI) (CA INDEX NAME)

PAGE 1-C

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PAGE 2-B

253342-12-0 HCAPLUS RN

Peptide nucleic acid, (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-dioxo-1)-2-(3,4-dioxo-1)-2-(3,4-d CNmethyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-

4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-

D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-

1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

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RN 253342-13-1 HCAPLUS

Peptide nucleic acid, (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (9CI) (CA INDEX NAME)

PAGE 3-A

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